High Energy and Momentum Resolved Photoemission Studies of Quasi-One-Dimensional Blue Bronze $K_{0.3}MoO_3$

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Outline

Introduction:

- ✓ Crystal structure
- ✓ Electronic structure
- ✓ Structural studies of Charge Density Waves

Experimental details:

- ✓ Photoelectron spectrometer

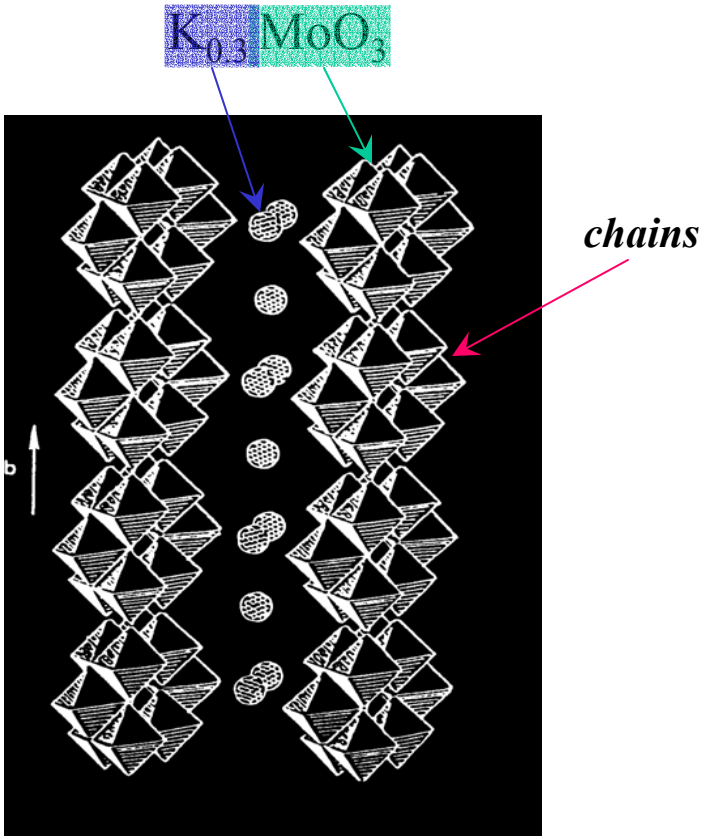
Experimental data:

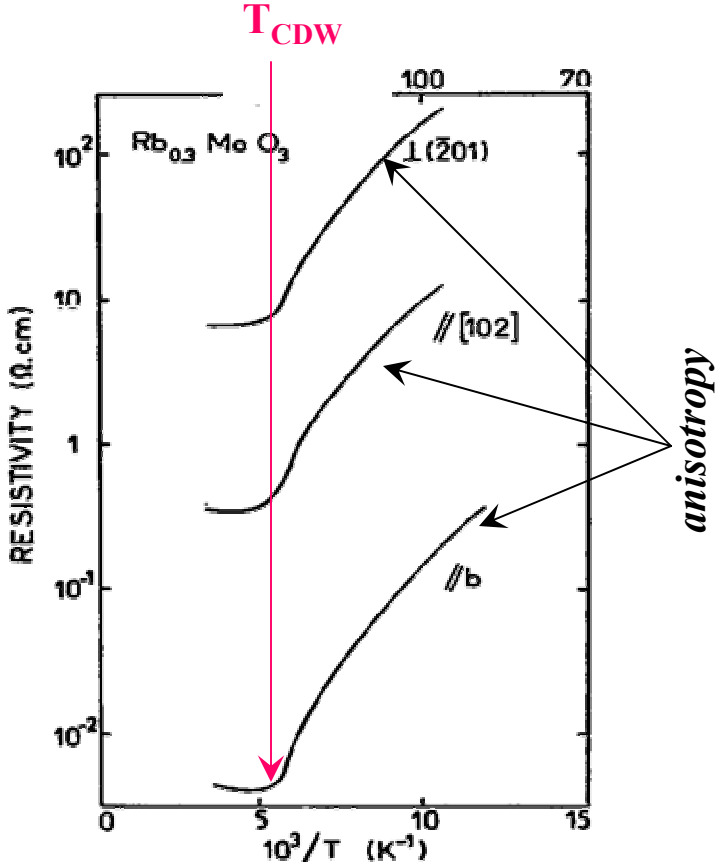
- ✓ Band structure of $K_{0.3}MoO_3$
- ✓ Fermi wave vectors versus temperature
- ✓ Commensurate to incommensurate CDW transition

Low dimensionality ⇒ *(i) Charge Density Waves (CDW), Peierls transitions*

(ii) Electron correlation effects

/Non-Fermi liquid behavior, spin-charge separation, HTC/



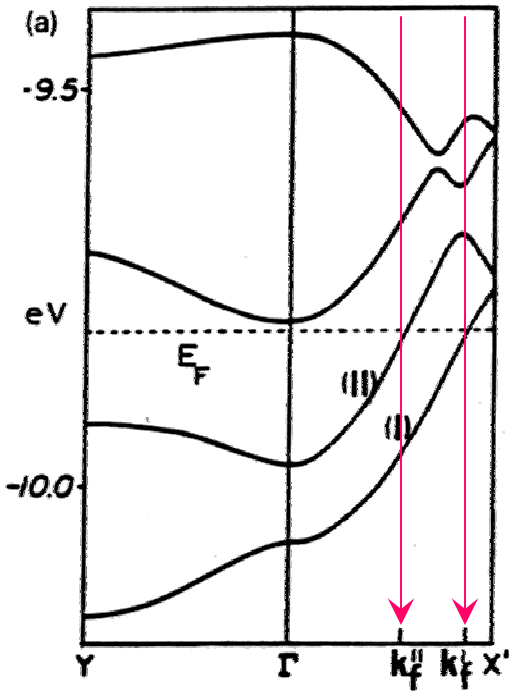


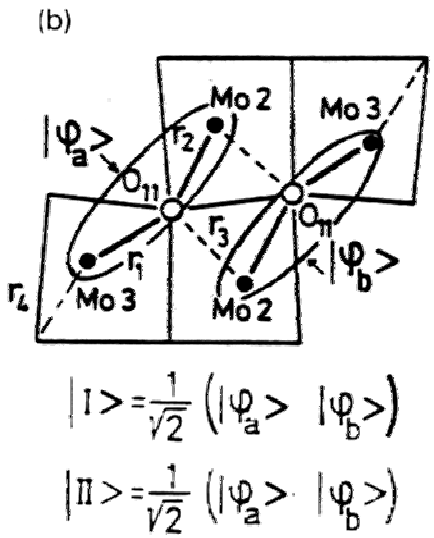
J.-P. Pouget et al., J. Physique Lett. 44, L113 (1973)

Electronic structure of $K_{0.3}MoO_3$

/tight-binding calculations/

M.-H. Whangbo and L.F. Schneemeyer, Inor. Chem. 25,2424 (1986)





Two chains per unit cell ⇒ two bands crossing the Fermi level

How many Charge Density Waves?

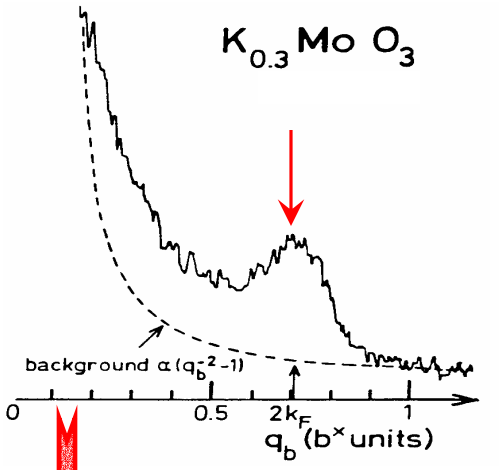
Structural studies of $K_{0.3}MoO_3$

/Single Charge Density Wave/

(i) Diffuse X-ray scattering

/$q_{CDW} = 2k_F b^x$/

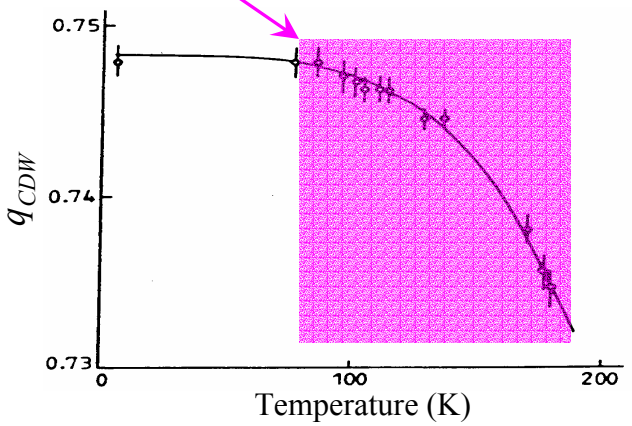
J.-P. Pougetet al.



(ii) Temperature dependent neutron scattering

/commensurate to incommensurate transition/

M.Sato, H. Fujishita and S.Hoshito,
J. Phys. C: Solid State phys., 16, L877 (1983)

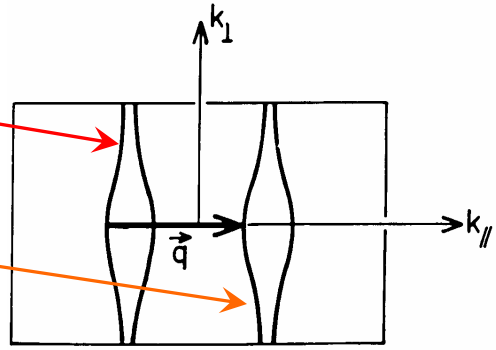


Nesting:

Fermi surface of the first band

is nested to the ***Fermi surface***

of the second band



CDW wave vector

$q_{CDW} : k_{F1}+k_{F2}$

Temperature dependence of CDW wave vector:

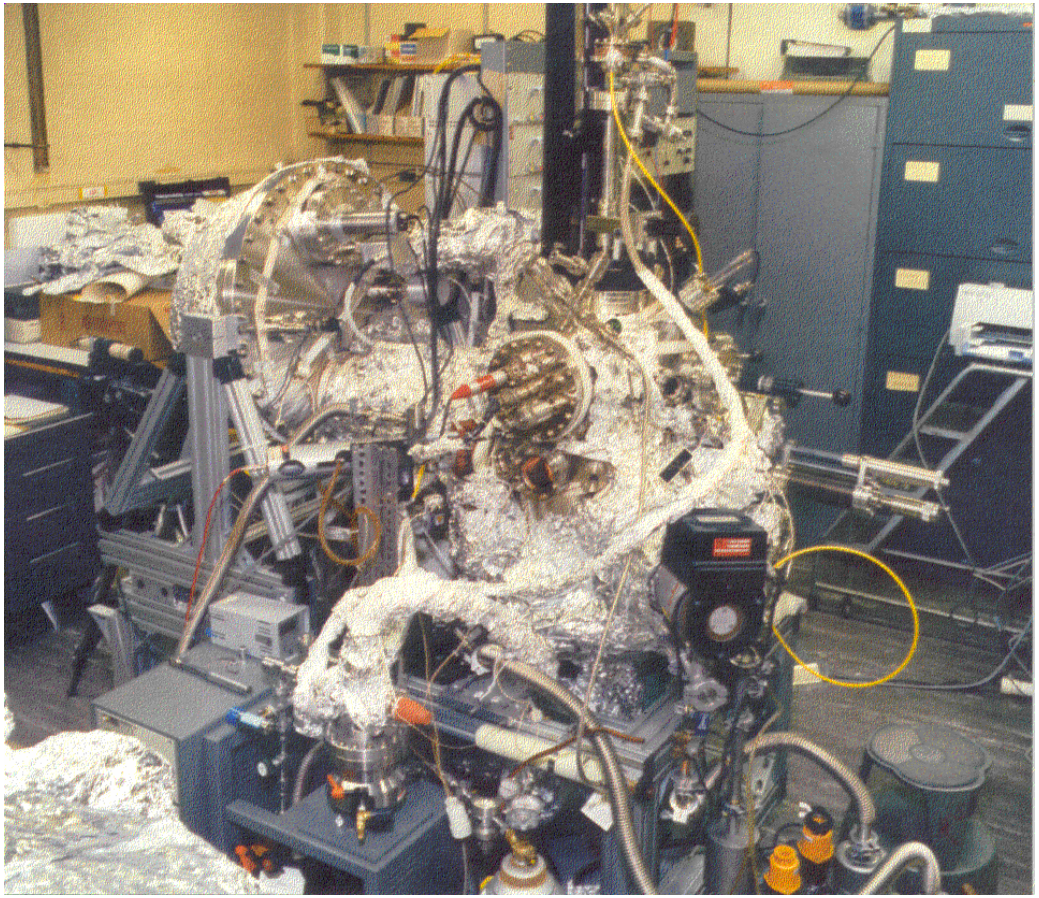
- Thermally activated charge transfer between bands crossing the Fermi level and third band above it */Pouget et al./*
- Shift of the chemical potential */Pouget & Nougera, Artemenko et al./*
- Hidden temperature dependence of the nesting vector */Intention of the present study/*

Goals of photoemission experiment:

- Direct monitoring k_{F1} and k_{F2}
- Temperature dependence of $(k_{F1}+k_{F2})$

Photoelectron Spectrometer
/Gammadata, SES-200/

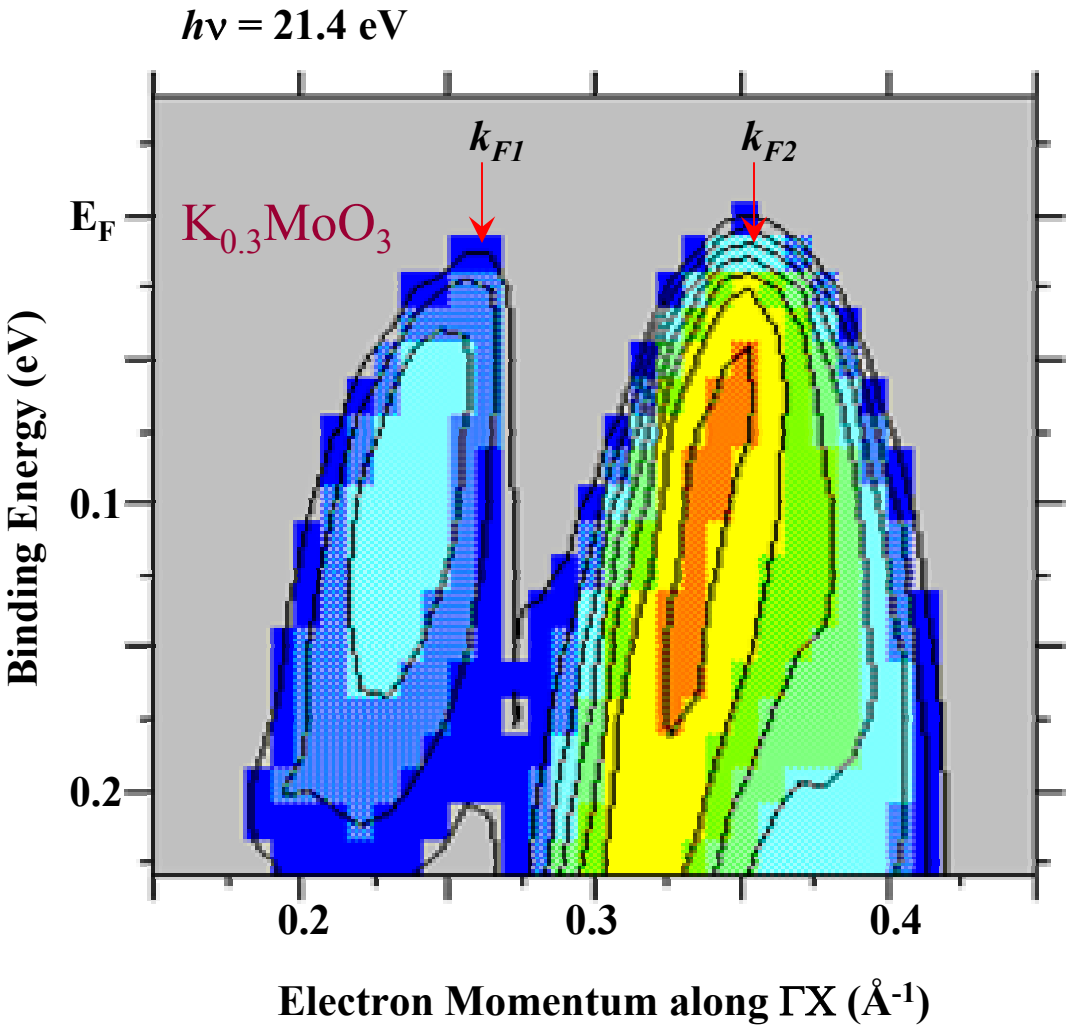
- ✓ *Multichannel detection in emission angle and kinetic energy*
- ✓ *Energy resolution ~ 10 meV*
- ✓ *Angle resolution ~ 0.2^{o}*
- ✓ *Base pressure ~ 2×10^{-11} Torr*



Presently located at the U13UB beamline at the National Synchrotron Light Source, BNL

Example of photoemission data

/3-D maps of photocurrent/



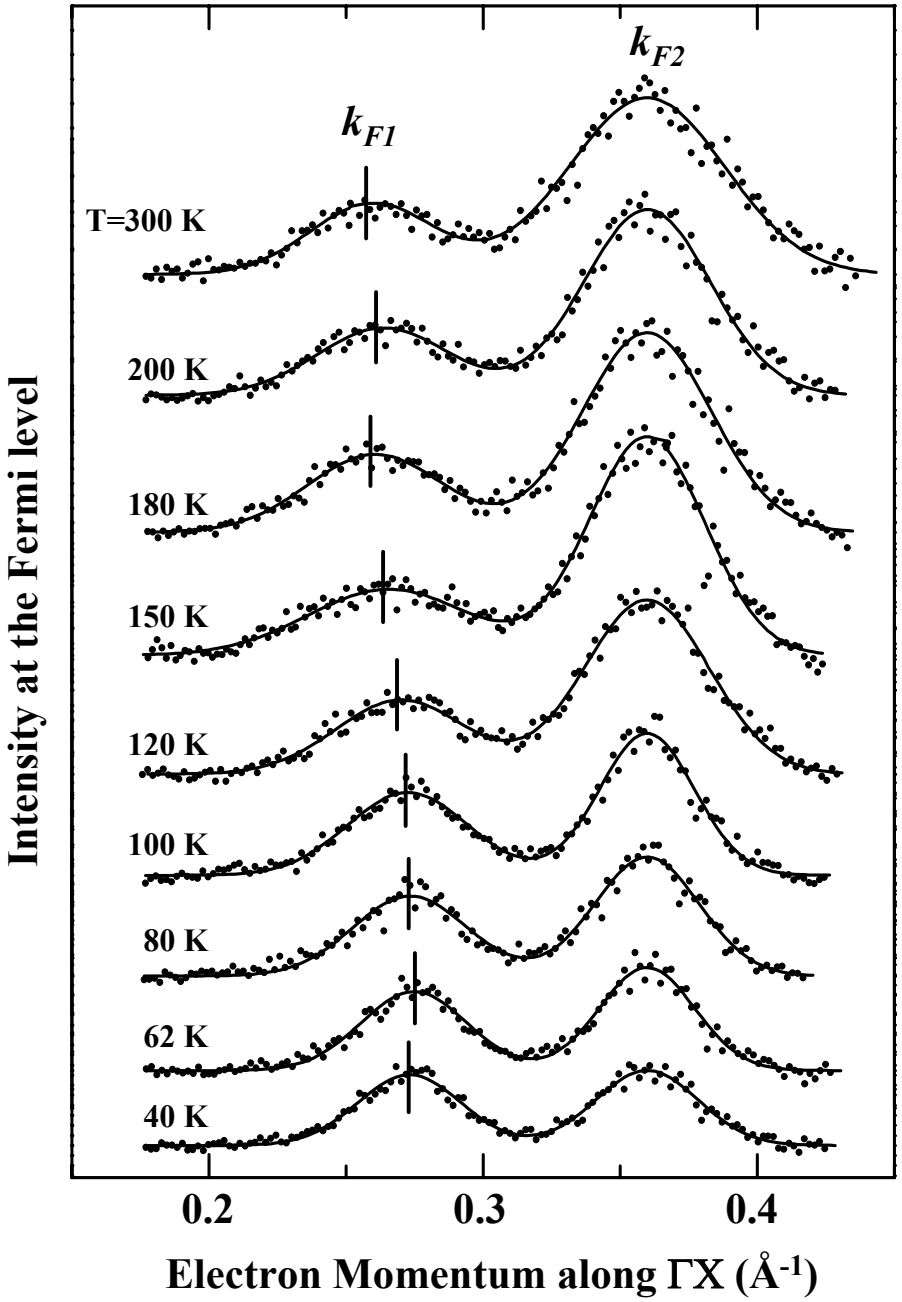
Experimental details:

Samples cleaved *in situ*

Liquid He cryostat provides temperatures from ~20 K to ~450 K

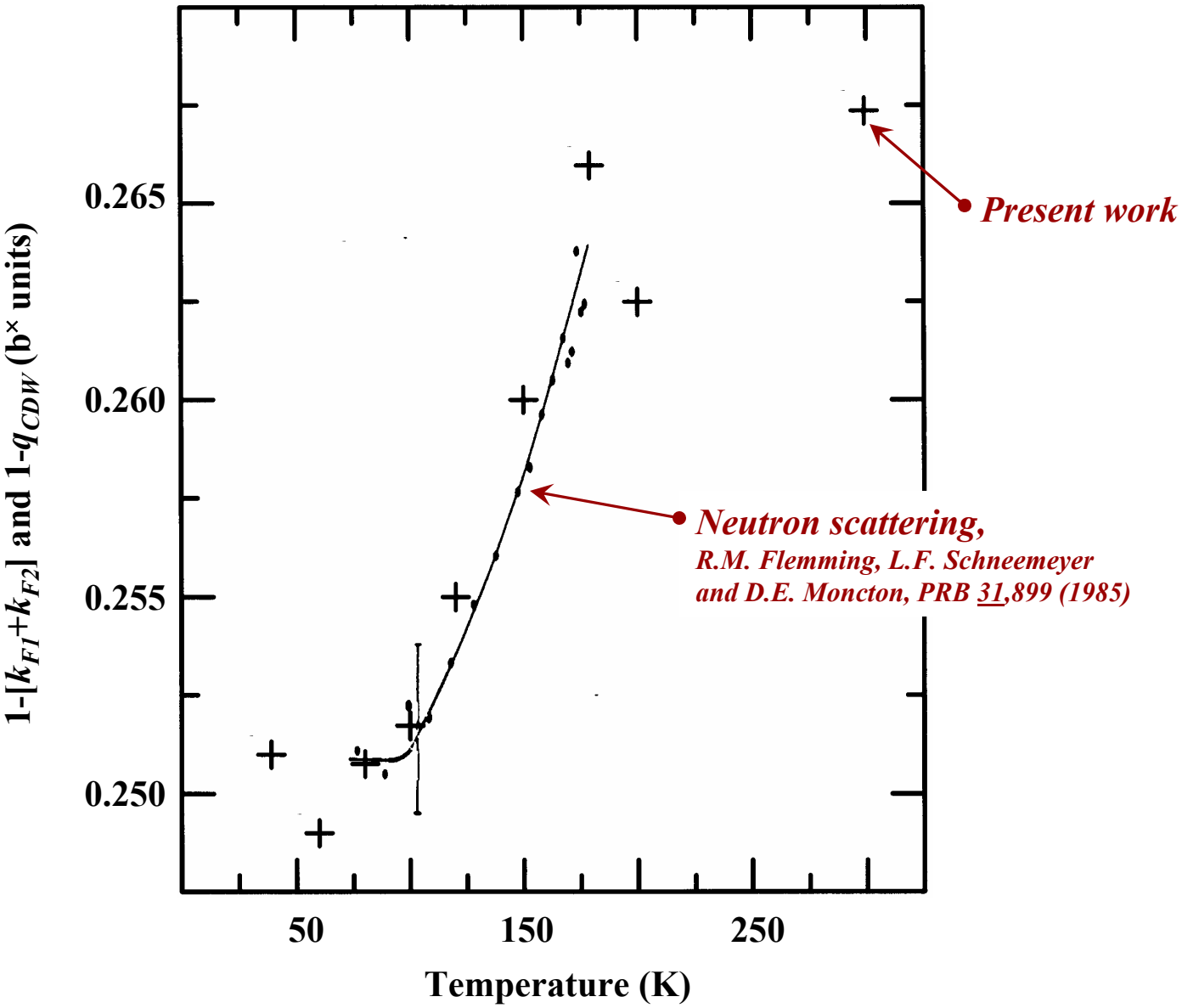
Temperature monitored with a help of OMEGA CY7 sensor

Momentum Distribution Curves at E_F



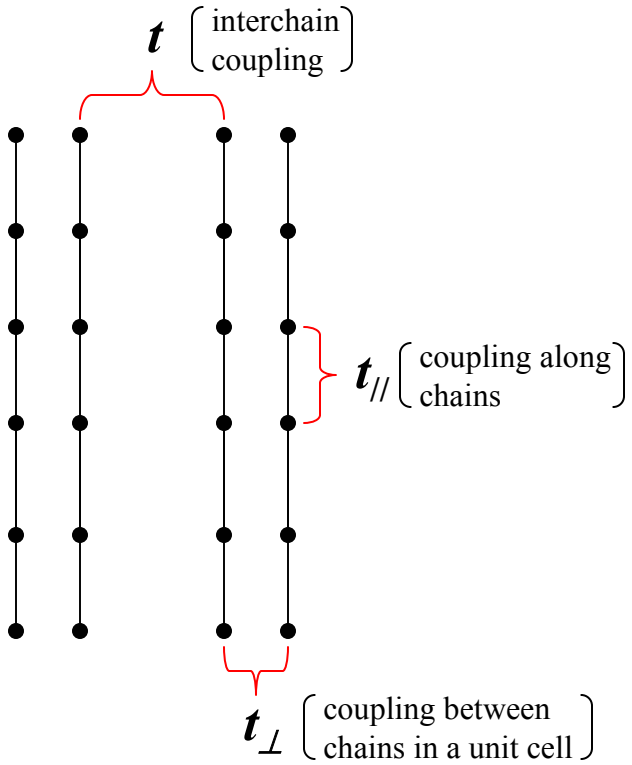
Commensurate to incommensurate CDW transition in $K_{0.3}MoO_3$

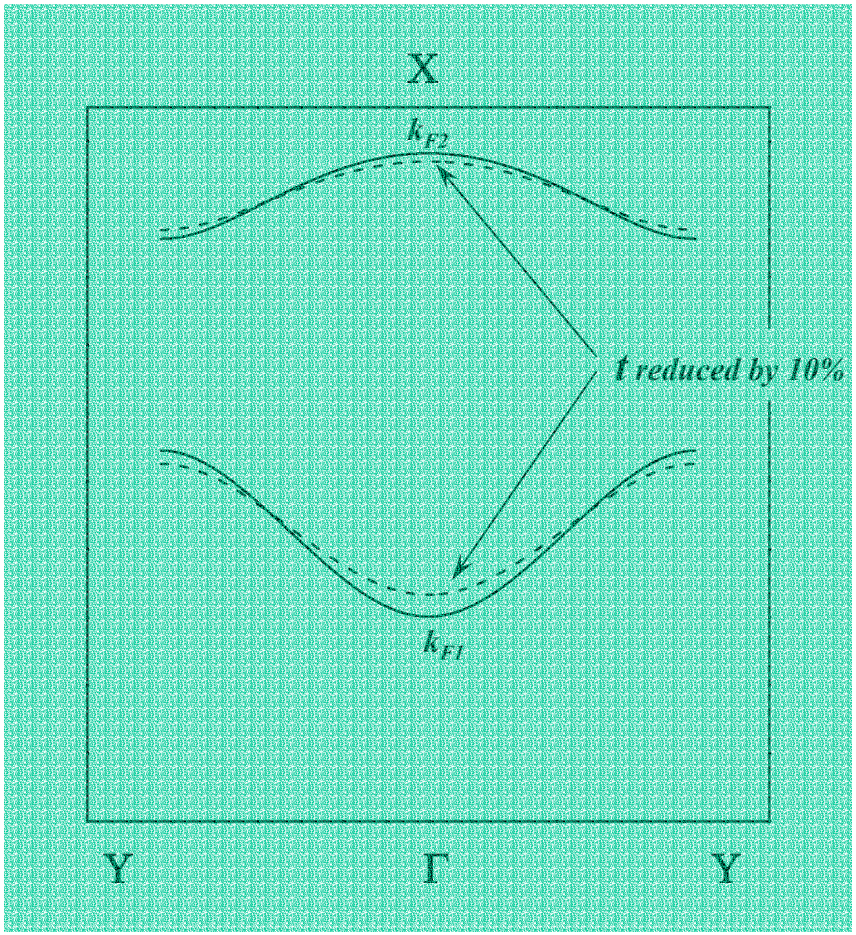
/comparing neutron scattering data with nesting vector measured in photoemission experiment/



Fermi surface of an array of coupled chains

/tight binding calculation/





Fermi surface is given by:

$$\mu = -2\cos(k_{//}) \pm (t_{\perp} + 2t_{\perp}\, t\cos(k_{\perp}) + t)$$